



Computational Toxicology Laboratory

WHAT IS THE HEALTH ISSUE?

- The safety of the food, air, and water from possible chemical contamination is a growing and documented public concern. CDC has developed a way to use biologically-based models to assess exposure, blood levels, and target tissue doses for specific chemical exposures, thus helping to determine the "safety" of the public's food, water, air, and other environmental medicine.
- Traditional chemical toxicity testing is extremely expensive and labor/time intensive.

WHAT HAS CDC ACCOMPLISHED?

The Computational Toxicology Laboratory uses computational toxicology methods--such as Quantitative Structure Activity Relationships (QSAR), Physiologically-based Pharmacokinetic (PBPK) modeling, and benchmark dose analyses methods as scientifically credible, timely, and cost-effective alternatives to traditional animal testing. Four main areas of public health applications have been identified:

- Hazardous Waste Sites: Chemical-specific PBPK models have been applied at hazardous waste sites to answer questions about "safety" of eating fish from local, polluted rivers and vegetables from home gardens.
- Children's Health: Child-based PBPK models for methylene chloride and tetrachloroethylene have been developed to determine if children are more sensitive to chemical exposures than adults.
- Research: International collaborations with TNO Nutrition and Food Research, Netherlands and the University of Georgia are investigating mechanisms of the interaction between multiple chemicals.
- Emergency Response and Terrorism: QSAR analyses have been conducted to predict toxicities of chemicals with no extant data which were part of an accidental release. The toxicological information was provided to the state department of health for an appropriate public health announcement.

WHAT ARE THE NEXT STEPS?

ATSDR is expanding its expertise in the field of QSAR and biologically-based modeling. Through collaborative efforts with CDC, the U.S. Environmental Protection Agency, and the National Toxicology Program, ATSDR is building capacity in computational toxicology to answer public health questions and to use as an important tool in public health and risk assessment.